Example 2e: User-Defined Material Properties – Input File

This example problem shows how users can specify their own constituent material properties for internal MAC/GMC 4.0 constitutive models through the code's input file. Note that Example Problems 1a and 1b touched on this subject. The present example includes ten materials in order to illustrate the input format for the elastic, Bodner-Partom, isotropic GVIPS, and incremental plasticity constitutive models (resulting in a large input file). To switch among the materials in separate code executions, the appropriate material number is specified under **`*RUC`**. A strain rate of 10^{-4}/sec. is employed, and results are generated for at a temperature of 500 °C. Another way in which the user can specify constituent material properties is through the use of a user-defined subroutine, which can calculate the material properties as a function of temperature or other quantity during code execution. This type of problem is illustrated in Example 2f. In the present example, the temperature-dependent or temperature-independent material properties are typed directly into the input file. It should be noted that the input file format for user-defined material properties is slightly different for each material constitutive model (as necessitated by the different material parameters needed for each constitutive model). See Section 2 of the MAC/GMC 4.0 Keywords Manual for more information on user-defined material properties.

MAC/GMC Input File: `example_2e.mac`

```
MAC/GMC 4.0 Example 2e - User-Defined Material Properties
*CONSTITUENTS
  NMATS=10
# -- Elastic; Temp-independent
  M=1 CMOD=6 MATID=U MATDB=1 &
    EL=58.E3,58.E3,0.20,0.20,24.17E3,6.3E-6,6.3E-6
# -- Elastic; Temp-dependent
  M=2 CMOD=6 MATID=U MATDB=1
   NTP=4
   TEM=18.,200.,400.,600.
   EA=45.6E3,43.5E3,40.6E3,29.0E3
   ET=45.6E3,43.5E3,40.6E3,29.0E3
   NUA=0.41,0.41,0.41,0.41
   NUT=0.41,0.41,0.41,0.41
   GA=16.154E3,15.429E3,14.400E3,10.286E3
   ALPA=4.5E-6,4.8E-6,5.1E-6,5.5E-6
   ALPT=4.5E-6,4.8E-6,5.1E-6,5.5E-6
# -- Bodner-Partom; Temp-independent
  M=3 CMOD=1 MATID=U MATDB=1 &
   EL=9.53E3,9.53E3,0.33,0.33,3.58E3,21.06E-6,21.06E-6  &
   VI=1.E4,49.,63.,300.,4.,1.
# -- Bodner-Partom; Temp-dependent
  M=4 CMOD=1 MATID=U MATDB=1
   NTP=2
   TEM=18.,700.
   EA=9.53E3,4.12E3
   ET=9.53E3,4.12E3
   NUA=0.41,0.41
   NUT=0.41,0.41
   GA=3.58E3,1.46E3
   ALPA=21.06E-6,28.92E-6
   ALPT=21.06E-6,28.92E-6
```

```
   V1=1.E4,1.E4
   V2=49.,49.
   V3=63.,63.
   V4=300.,300.
   V5=4.,2.5
   V6=1.,1.
# -- Isotropic GVIPS; Temp-independent
  M=5 CMOD=4 MATID=U MATDB=1  &
   EL=14009.,14009.,0.365,0.365,5131.5,5.862E-6,5.862E-6 &
   VI=0.000999275,44.960,1.679E-07,2.494561E-05,0.05, &
      3.3,1.8,1.35,0.85,3.0183E-7,0.001
# -- Isotropic GVIPS; Temp-dependent
  M=6 CMOD=4 MATID=U MATDB=1
   NTP=6
   TEM=25.,300.,482.,565.,650.,704.
   EA=16.5506E+03,15.644E+03,14.009E+03,12.968E+03,11.702E+03,10.793E+03
   ET=16.5506E+03,15.644E+03,14.009E+03,12.968E+03,11.702E+03,10.793E+03
   NUA=0.365,0.365,0.365,0.365,0.365,0.365
   NUT=0.365,0.365,0.365,0.365,0.365,0.365
   GA=6062.491,5730.403,5131.502,4750.183,4286.477,3953.480
   ALPA=4.2921E-06,5.116E-06,5.862E-06,6.271E-06,6.741E-06,7.07E-06
   ALPT=4.2921E-06,5.116E-06,5.862E-06,6.271E-06,6.741E-06,7.07E-06
   V1=99.927,20.015,0.000999275,8.499E-08,8.E-8,1.02973E-12
   V2=149.964,111.965,44.960,4.786,0.8499,0.10877
   V3=0.,0.,1.679E-07,1.685E-07,0.000001,0.00006
   V4=9.992748E-06,1.493836E-05,2.494561E-05,7.048586E-05, &
      8.498912E-05,9.224075E-05
   V5=0.05,0.05,0.05,0.05,0.05,0.05
   V6=3.3,3.3,3.3,3.3,3.3,3.3
   V7=1.8,1.8,1.8,1.8,1.8,1.8
   V8=1.35,1.35,1.35,1.35,1.35,1.35
   V9=0.8498912,0.8498912,0.8498912,0.8498912,0.8498912,0.8498912
   V10=1.7984E-8,3.6484E-8,3.0183E-7,3.5965E-7,1.5246E-7,1.3429E-7
   V11=0.001,0,0,0,0,0
# -- Bilinear plasticity; Temp-independent
  M=7 CMOD=21 MATID=U MATDB=1 &
   EL=10000.,10000.,0.326,0.326,3770.,12.00E-6,12.00E-6 &
   NP=1 VI=5.08,13.1,0.15
# -- Bilinear plasticity; Temp-dependent
  M=8 CMOD=21 MATID=U MATDB=1
   NTP=3
   TEM=21.,400.,800.
   EA=10000.,9000.,7300.
   ET=10000.,9000.,7300.
   NUA=0.326,0.351,0.345
   NUT=0.326,0.351,0.345
   GA=3771.,3331.,2714.
   ALPA=12.00E-6,13.50E-6,22.72E-6
   ALPT=12.00E-6,13.50E-6,22.72E-6
   NP=1
   V1=5.08,4.21,3.05
   V2=13.1,10.7,5.10
   V3=0.15,0.15,0.15
# -- Point-wise plasticity; Temp-independent
  M=9 CMOD=21 MATID=U MATDB=1 &
   EL=10000.,10000.,0.326,0.326,3770.,12.00E-6,12.00E-6 &
   NP=3 VI=4.20,6.13,6.60,13.1,0.004,0.01,0.15
```

```
# -- Point-wise plasticity; Temp-dependent
  M=10 CMOD=21 MATID=U MATDB=1
   NTP=3
   TEM=21.,400.,800.
   EA=10000.,9000.,7300.
   ET=10000.,9000.,7300.
   NUA=0.326,0.351,0.345
   NUT=0.326,0.351,0.345
   GA=3771.,3331.,2714.
   ALPA=12.00E-6,13.50E-6,22.72E-6
   ALPT=12.00E-6,13.50E-6,22.72E-6
   NP=3
   V1=4.20,3.81,3.05
   V2=6.13,4.77,3.69
   V3=6.60,5.10,3.90
   V4=13.1,9.70,5.10
   V5=0.004,0.004,0.004
   V6=0.01,0.01,0.01
   V7=0.15,0.15,0.15
*RUC
# -- Alter value of M=* to change simulated material
  MOD=1 M=1
*MECH
  LOP=1
  NPT=2 TI=0.,200. MAG=0.,0.02 MODE=1
*THERM
  NPT=2 TI=0.,200. TEMP=500.,500.
*SOLVER
  METHOD=1 NPT=2 TI=0.,200. STP=0.1 ITMAX=20 ERR=1.E-6
*PRINT
  NPL=6
*XYPLOT
  FREQ=1
  MACRO=1
   NAME=example_2e X=1 Y=7
  MICRO=0
*END
```

Annotated Input Data

1) Flags: None

2) Constituent materials (***CONSTITUENTS**) [KM_2]:

Number of materials:	10	(NMATS=10)
Materials:	User-Defined	(MATID=U)
Material property source:	Read from input file	(MATDB=1)

Constitutive models:

Linear Elastic (CMOD=6)

```
# -- Elastic; Temp-independent
  M=1 CMOD=6 MATID=U MATDB=1 &
    EL=58.E3,58.E3,0.20,0.20,24.17E3,6.3E-6,6.3E-6
# -- Elastic; Temp-dependent
```

```
M=2 CMOD=6 MATID=U MATDB=1
 NTP=4
 TEM=18.,200.,400.,600.
 EA=45.6E3,43.5E3,40.6E3,29.0E3
 ET=45.6E3,43.5E3,40.6E3,29.0E3
 NUA=0.41,0.41,0.41,0.41
 NUT=0.41,0.41,0.41,0.41
 GA=16.154E3,15.429E3,14.400E3,10.286E3
 ALPA=4.5E-6,4.8E-6,5.1E-6,5.5E-6
 ALPT=4.5E-6,4.8E-6,5.1E-6,5.5E-6
```

The simplest constitutive model for which to input user-defined material properties is the linearly elastic model (`CMOD=6`). Since the material deformation is treated as linearly elastic, all that is needed is the thermo-elastic material properties. The standard order for the material properties is: E_A, E_T, ν_A, ν_T, G_A, α_A, α_T. As shown above, for temperature-independent material properties, these properties are simply listed as `EL=`..., on the same line in the input file. For temperature-dependent material properties, the number of input temperatures (`NTP=4`) is placed on a separate line, followed by a separate line specifying the input temperatures (`TEM=`...). Then, each of the seven material properties is placed on its own separate line, with the values at each of the input temperatures listed.

Bodner-Partom (`CMOD=1`)

```
# -- Bodner-Partom; Temp-independent
  M=3 CMOD=1 MATID=U MATDB=1 &
   EL=9.53E3,9.53E3,0.33,0.33,3.58E3,21.06E-6,21.06E-6  &
   VI=1.E4,49.,63.,300.,4.,1.
# -- Bodner-Partom; Temp-dependent
  M=4 CMOD=1 MATID=U MATDB=1
   NTP=2
   TEM=18.,700.
   EA=9.53E3,4.12E3
   ET=9.53E3,4.12E3
   NUA=0.41,0.41
   NUT=0.41,0.41
   GA=3.58E3,1.46E3
   ALPA=21.06E-6,28.92E-6
   ALPT=21.06E-6,28.92E-6
   V1=1.E4,1.E4
   V2=49.,49.
   V3=63.,63.
   V4=300.,300.
   V5=4.,2.5
   V6=1.,1.
```

For the Bodner-Partom viscoplastic constitutive model, the user-defined elastic material properties are specified in the same manner as for the elastic material constitutive model. Now, however, six viscoplastic material properties must also be specified. In the case of temperature-independence, these six material parameters are simply listed on the same line as the elastic properties as `VI=`.... In the case of temperature-dependence, each viscoplastic material property is placed on its own line as shown above. Obviously, the order in which these viscoplastic material properties is specified is important as the code must know how to interpret the input data. For the Bodner-Partom model, this order is: D_0, Z_0 ,Z_1 , m, n, q . This order, as well as the proper order for the other MAC/GMC 4.0 internal constitutive models, is described in Section 2 of the MAC/GMC 4.0 Keywords Manual.

Isotropic GVIPS (CMOD=4)

```
# -- Isotropic GVIPS; Temp-independent
  M=5 CMOD=4 MATID=U MATDB=1  &
   EL=14009.,14009.,0.365,0.365,5131.5,5.862E-6,5.862E-6 &
   VI=0.000999275,44.960,1.679E-07,2.494561E-05,0.05, &
      3.3,1.8,1.35,0.85,3.0183E-7,0.001
# -- Isotropic GVIPS; Temp-dependent
  M=6 CMOD=4 MATID=U MATDB=1
   NTP=6
   TEM=25.,300.,482.,565.,650.,704.
   EA=16.5506E+03,15.644E+03,14.009E+03,12.968E+03,11.702E+03,10.793E+03
   ET=16.5506E+03,15.644E+03,14.009E+03,12.968E+03,11.702E+03,10.793E+03
   NUA=0.365,0.365,0.365,0.365,0.365,0.365
   NUT=0.365,0.365,0.365,0.365,0.365,0.365
   GA=6062.491,5730.403,5131.502,4750.183,4286.477,3953.480
   ALPA=4.2921E-06,5.116E-06,5.862E-06,6.271E-06,6.741E-06,7.07E-06
   ALPT=4.2921E-06,5.116E-06,5.862E-06,6.271E-06,6.741E-06,7.07E-06
   V1=99.927,20.015,0.000999275,8.499E-08,8.E-8,1.02973E-12
   V2=149.964,111.965,44.960,4.786,0.8499,0.10877
   V3=0.,0.,1.679E-07,1.685E-07,0.000001,0.00006
   V4=9.992748E-06,1.493836E-05,2.494561E-05,7.048586E-05, &
      8.498912E-05,9.224075E-05
   V5=0.05,0.05,0.05,0.05,0.05,0.05
   V6=3.3,3.3,3.3,3.3,3.3,3.3
   V7=1.8,1.8,1.8,1.8,1.8,1.8
   V8=1.35,1.35,1.35,1.35,1.35,1.35
   V9=0.8498912,0.8498912,0.8498912,0.8498912,0.8498912,0.8498912
   V10=1.7984E-8,3.6484E-8,3.0183E-7,3.5965E-7,1.5246E-7,1.3429E-7
   V11=0.001,0,0,0,0,0
```

As with Bodner-Partom viscoplasticity, employing user-defined material properties with the GVIPS constitutive model requires specification of viscoplastic material properties in addition to the elastic properties. Now, instead of six viscoplastic parameters, there are eleven. As mentioned previously, the correct order for specification of these eleven properties is discussed in the MAC/GMC 4.0 Keywords Manual in Section 2.

Incremental Plasticity (CMOD=21)

```
# -- Bilinear plasticity; Temp-independent
  M=7 CMOD=21 MATID=U MATDB=1 &
   EL=10000.,10000.,0.326,0.326,3770.,12.00E-6,12.00E-6 &
   NP=1 VI=5.08,13.1,0.15
# -- Bilinear plasticity; Temp-dependent
  M=8 CMOD=21 MATID=U MATDB=1
   NTP=3
   TEM=21.,400.,800.
   EA=10000.,9000.,7300.
   ET=10000.,9000.,7300.
   NUA=0.326,0.351,0.345
   NUT=0.326,0.351,0.345
   GA=3771.,3331.,2714.
   ALPA=12.00E-6,13.50E-6,22.72E-6
   ALPT=12.00E-6,13.50E-6,22.72E-6
   NP=1
   V1=5.08,4.21,3.05
```

```
   V2=13.1,10.7,5.10
   V3=0.15,0.15,0.15
# -- Point-wise plasticity; Temp-independent
  M=9 CMOD=21 MATID=U MATDB=1 &
   EL=10000.,10000.,0.326,0.326,3770.,12.00E-6,12.00E-6 &
   NP=3 VI=4.20,6.13,6.60,13.1,0.004,0.01,0.15
# -- Point-wise plasticity; Temp-dependent
  M=10 CMOD=21 MATID=U MATDB=1
   NTP=3
   TEM=21.,400.,800.
   EA=10000.,9000.,7300.
   ET=10000.,9000.,7300.
   NUA=0.326,0.351,0.345
   NUT=0.326,0.351,0.345
   GA=3771.,3331.,2714.
   ALPA=12.00E-6,13.50E-6,22.72E-6
   ALPT=12.00E-6,13.50E-6,22.72E-6
   NP=3
   V1=4.20,3.81,3.05
   V2=6.13,4.77,3.69
   V3=6.60,5.10,3.90
   V4=13.1,9.70,5.10
   V5=0.004,0.004,0.004
   V6=0.01,0.01,0.01
   V7=0.15,0.15,0.15
```

The incremental plasticity constitutive model is a special case in terms of specifying user-defined material properties. The implementation of this model with MAC/GMC 4.0 allows the constituent material's response to be defined by a number of stress – total strain point pairs that can be taken directly from experimental data for a material. Note that this simplifies the input compared to specification of stress – inelastic strain point pairs. A maximum of nine such pairs is permitted for each temperature. As shown above, the number of these stress-strain point pairs employed by the user must be specified as `NP=*`. This is the number of stress-strain pairs that are specified in addition to the material's yield stress. In the case of temperature-independence, `NP=*` is placed on the same line, while for temperature-dependence, `NP=*` is placed on its own line. The smallest permitted value for NP=* is 1, which corresponds to bilinear plasticity. In this case, three plastic material parameters are specified, the first being the yield stress, followed by the stress and strain corresponding to one post-yield stress-strain pair. The material response is bilinear in that, at stresses below yield, the stress-strain response is linearly elastic, while after yielding, the response follows a linear path defined by the yield stress – total strain point and the single specified post-yield stress – total strain pair. The case where NP > 1, is referred to as point-wise plasticity, as the post-yield material response will follow a piece-wise linear path defined by the (up to nine) specified stress – total strain point pairs. The order for the user-defined properties for point-wise plasticity is:

$$\sigma_Y,\ \sigma_1,\ \sigma_2,\ ...,\sigma_{NP},\ \varepsilon_1,\ \varepsilon_2,\ ...,\ \varepsilon_{NP}$$

where σ_Y is the yield stress and $\sigma_i - \varepsilon_i$ are the stress – total strain points. As indicated above, this ordering holds true for temperature-dependent material properties as well, as each value on a particular line represents a different temperature. For instance, `V1=4.20,3.81,3.05` are the values of the yield stress at the three input temperatures (21., 400., and 800. °C), `V2=6.13,4.77,3.69` are the stress values (σ_1) of the first stress-strain point at the three input temperatures, and V5=0.004,0.004,0.004 are the total strain values (ε_1) of the first stress-strain point at the three input temperatures. Note that the total number of incremental plasticity material parameters is 2×NP+1.

3) Analysis type (***RUC**) → Repeating Unit Cell Analysis [KM_3]:

Analysis model:	Monolithic material	(MOD=1)
Material assignment:	Each constituent successively	(M=*)

4) Loading:

a) Mechanical (***MECH**) [KM_4]:

Loading option:	1	(LOP=1)
Number of points:	2	(NPT=2)
Time points:	0., 200. sec.	(TI=0.,200.)
Load magnitude:	0., 0.02	(MAG=0.,0.02)
Loading mode:	strain control	(MODE=1)

b) Thermal (***THERM**) [KM_4]:

Number of points:	2	(NPT=2)
Time points:	0., 200. sec.	(TI=0.,200.)
Temperature points:	500., 500.	(TEMP=500.,500.)

c) Time integration (***SOLVER**) [KM_4]:

Time integration method:	Forward Euler	(METHOD=1)
Number of time points:	2	(NPT=2)
Time points:	0., 20. sec.	(TI=0.,20.)
Time step sizes:	0.1 sec.	(STP=0.1)
Max. number of iterations	20	(ITMAX=20)
Max. permitted error fraction	$1.\times10^{-6}$	(ERR=1.E-6)

☞ Note: While ITMAX=20 and ERR=1.E-6 are present in the input file for all ten cases executed in this example problem, these data are required only for the incremental plasticity cases. As mentioned in Example 2c, if oscillations occur in the results, a smaller value for ERR and/or a smaller time step should be employed.

5) Damage and Failure: None

6) Output:

a) Output file print level (***PRINT**) [KM_6]:

Print level:	6	(NPL=6)

b) x-y plots (***XYPLOT**) [KM_6]:

Frequency:	1	(FREQ=1)
Number of macro plots:	1	(MACRO=1)
Macro plot name:	example_2e	(NAME=example_2e)
Macro plot x-y quantities:	ε_{11}, σ_{11}	(X=1 Y=7)
Number of micro plots:	0	(MICRO=0)

7) End of file keyword: (***END**)

Results

The results for this example problem are plotted in Figure 2.5 and Figure 2.6. When temperature-dependent material properties are specified (as they are for material numbers 2, 4, 6, 8, and 10), MAC/GMC 4.0 uses linear interpolation to determine the properties at temperature between those specified. When temperature-independent material properties are specified, these properties are employed regardless of the current temperature during the simulation. Since the stress-strain results presented here were generated at a temperature of 500 °C, significant differences are evident between the temperature-dependent and temperature-independent materials for each constitutive model.

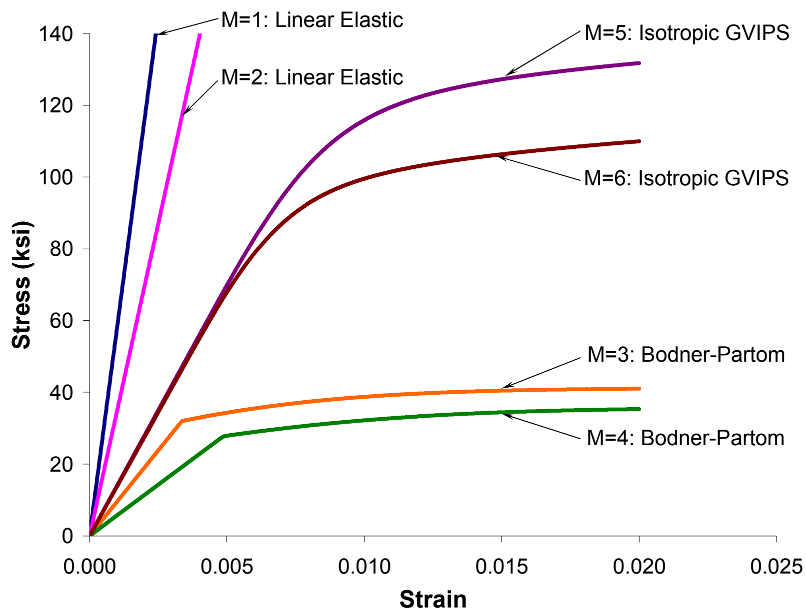

Figure 2.5 Example 2e: plots of the tensile stress-strain response of the first 6 user-defined materials at 500 °C.

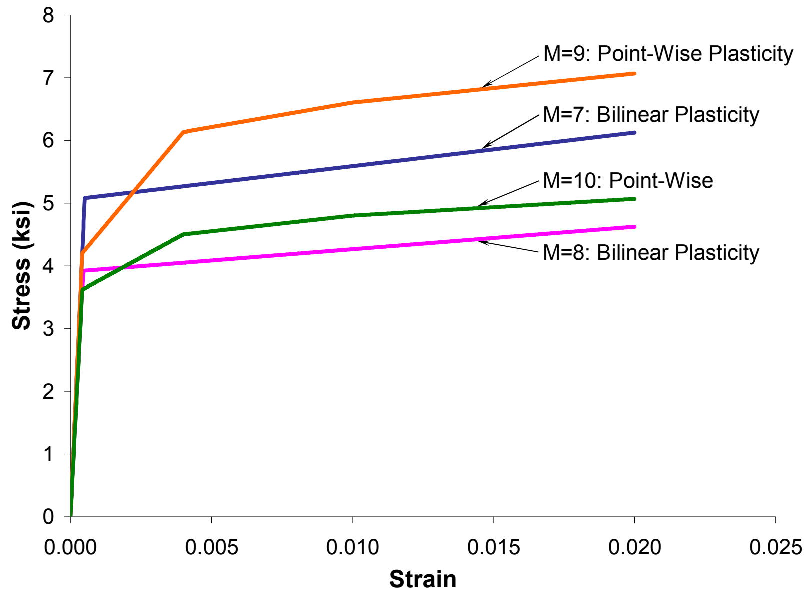

Figure 2.6 Example 2e: plots of the tensile stress-strain response of the incremental plasticity user-defined materials at 500 °C.